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Chiral crystallization of cis-2,3-dichloro-buth-2-e-e-1,4-diol

Lodochnikova O., Latypova L., Khakimov R., Kurbangalieva A., Krivolapov D., Litvinov I.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

The X-ray diffraction study of cis-2,3-dichlorobuth-2-ene-1,4-diol (3) obtained by the reduction of 3,4-dichloro-5-ethoxy- and 5-isopropoxi-2(5H)- furanones with lithium aluminum hydride is performed. The crystals of compound 3 are trigonal: a = b = 15.746(9) Å, c = 6.848(4) Å; V = 1470.5(15) Å3, space group P31, Z = 9 (three independent molecules). Independent molecules have identical planar conformation, and hydroxyl groups are located on different sides of the multiple bond plane. The supramolecular motif of the crystal is spirals about the threefold screw axes; the neighboring spirals are linked by OH.O hydrogen bonds. © 2013 Pleiades Publishing, Ltd.

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Keywords

chiral crystallization, cis-2,3-dichlorobuth-2-ene-1,4-diol, hydrogen bonds, supramolecular structure, X-ray diffraction study